10540421

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NEWS 1		Web Page for STN Seminar Schedule - N. America
NEWS 2	OCT 02	CA/CAplus enhanced with pre-1907 records from Chemisches Zentralblatt
NEWS 3	OCT 19	BEILSTEIN updated with new compounds
NEWS 4	NOV 15	Derwent Indian patent publication number format enhanced
NEWS 5	NOV 19	WPIX enhanced with XML display format
NEWS 6	NOV 30	ICSD reloaded with enhancements
NEWS 7	DEC 04	LINPADOCDB now available on STN
NEWS 8	DEC 14	BEILSTEIN pricing structure to change
NEWS 9	DEC 17	USPATOLD added to additional database clusters
NEWS 10	DEC 17	IMSDRUGCONF removed from database clusters and STN
NEWS 11	DEC 17	DGENE now includes more than 10 million sequences
NEWS 12	DEC 17	TOXCENTER enhanced with 2008 MeSH vocabulary in MEDLINE segment
NEWS 13	DEC 17	MEDLINE and LMEDLINE updated with 2008 MeSH vocabulary
NEWS 14	DEC 17	CA/CAplus enhanced with new custom IPC display formats
NEWS 15	DEC 17	STN Viewer enhanced with full-text patent content from USPATOLD
NEWS 16	JAN 02	STN pricing information for 2008 now available
NEWS 17	JAN 16	CAS patent coverage enhanced to include exemplified prophetic substances
NEWS 18	JAN 28	USPATFULL, USPAT2, and USPATOLD enhanced with new custom IPC display formats
NEWS 19	JAN 28	MARPAT searching enhanced
NEWS 20	JAN 28	USGENE now provides USPTO sequence data within 3 days of publication
NEWS 21	JAN 28	TOXCENTER enhanced with reloaded MEDLINE segment
NEWS 22	JAN 28	MEDLINE and LMEDLINE reloaded with enhancements
NEWS 23	FEB 08	STN Express, Version 8.3, now available
NEWS 24	FEB 20	PCI now available as a replacement to DPCI
NEWS 25	FEB 25	IFIREF reloaded with enhancements
NEWS 26	FEB 25	IMSPRODUCT reloaded with enhancements
NEWS 27	FEB 29	WPINDEX/WPIDS/WPIX enhanced with ECLA and current U.S. National Patent Classification

NEWS EXPRESS FEBRUARY 08 CURRENT WINDOWS VERSION IS V8.3,
AND CURRENT DISCOVER FILE IS DATED 20 FEBRUARY 2008

NEWS HOURS STN Operating Hours Plus Help Desk Availability

Updated Search

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```
 NEWS LOGIN    Welcome Banner and News Items
 NEWS IPC8     For general information regarding STN implementation of IPC 8

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* * * * * * * * * * * * * * * STN  Columbus  * * * * * * * * * * * * * * *

FILE 'HOME' ENTERED AT 22:11:52 ON 11 MAR 2008

=> file reg
COST IN U.S. DOLLARS                                SINCE FILE      TOTAL
                                                       ENTRY    SESSION
FULL ESTIMATED COST                                     0.21       0.21

FILE 'REGISTRY' ENTERED AT 22:11:58 ON 11 MAR 2008
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STRUCTURE FILE UPDATES:   10 MAR 2008  HIGHEST RN 1007341-18-5
DICTIONARY FILE UPDATES:  10 MAR 2008  HIGHEST RN 1007341-18-5

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TSCA INFORMATION NOW CURRENT THROUGH January 9, 2008.

  Please note that search-term pricing does apply when
  conducting SmartSELECT searches.

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predicted properties as well as tags indicating availability of
experimental property data in the original document.  For information
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http://www.cas.org/support/stngen/stndoc/properties.html

=>
Uploading C:\Documents and Settings\brobinson1\My Documents\stnweb\Queries\asdgk.str

L1      STRUCTURE UPLOADED

=> d l1
L1 HAS NO ANSWERS
L1              STR
*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***
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Updated Search

10540421

Structure attributes must be viewed using STN Express query preparation.

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=> s l1
SAMPLE SEARCH INITIATED 22:14:41 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED -      303 TO ITERATE

100.0% PROCESSED      303 ITERATIONS                                0 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:  ONLINE   **COMPLETE**
                        BATCH    **COMPLETE**
PROJECTED ITERATIONS:         5016 TO     7104
PROJECTED ANSWERS:               0 TO        0

L2            0 SEA SSS SAM L1

=> s l1 full
THE ESTIMATED SEARCH COST FOR FILE 'REGISTRY' IS 177.90 U.S. DOLLARS
DO YOU WANT TO CONTINUE WITH THIS REQUEST? (Y)/N or END:y
FULL SEARCH INITIATED 22:14:45 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED -     6538 TO ITERATE

100.0% PROCESSED     6538 ITERATIONS                                2 ANSWERS
SEARCH TIME: 00.00.01

L3            2 SEA SSS FUL L1

=> file hcaplus
COST IN U.S. DOLLARS                                SINCE FILE      TOTAL
                                                       ENTRY    SESSION
FULL ESTIMATED COST                                   180.20     180.41

FILE 'HCAPLUS' ENTERED AT 22:14:49 ON 11 MAR 2008
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FILE COVERS 1907 - 11 Mar 2008  VOL 148 ISS 11
FILE LAST UPDATED: 10 Mar 2008  (20080310/ED)

New CAS Information Use Policies, enter HELP USAGETERMS for details.

 This file contains CAS Registry Numbers for easy and accurate
 substance identification.
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Updated Search

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=> s l3
L4            2 L3

=> s l4 and shinya, y?/au
             58 SHINYA, Y?/AU
L5            0 L4 AND SHINYA, Y?/AU

=> s l4 and watanabe, t?/au
          22474 WATANABE, T?/AU
L6            2 L4 AND WATANABE, T?/AU

=> d l6, ibib abs hitstr, 1-2

L6   ANSWER 1 OF 2  HCAPLUS  COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER:         2004:872791  HCAPLUS
DOCUMENT NUMBER:          141:350046
TITLE:                    Preparation of novel crystal of fluorobenzamide
                          derivative
INVENTOR(S):              Yoshida, Shinya; Watanabe, Toshihiro;
                          Marumo, Kiyotaka; Yamaguchi, Sou
PATENT ASSIGNEE(S):       Yamanouchi Pharmaceutical Co., Ltd., Japan
SOURCE:                   PCT Int. Appl., 25 pp.
                          CODEN: PIXXD2
DOCUMENT TYPE:            Patent
LANGUAGE:                 Japanese
FAMILY ACC. NUM. COUNT:   1
PATENT INFORMATION:

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     WO 2004089933        A1    20041021    WO 2004-JP4794         20040401
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             CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD,
             GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC,
             LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI,
             NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY,
             TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
         RW: BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ,
             BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE,
             ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI,
             SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN,
             TD, TG
     CA 2519882           A1    20041021    CA 2004-2519882        20040401
     EP 1609788           A1    20051228    EP 2004-725182         20040401
         R:  AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,
             IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, PL, SK, HR
     CN 1771245           A     20060510    CN 2004-80009451       20040401
     IN 2005DN04378       A     20070105    IN 2005-DN4378         20050927
     MX 2005PA10603       A     20060725    MX 2005-PA10603        20050930
     US 2007129357        A1    20070607    US 2005-552019         20051003
PRIORITY APPLN. INFO.:                       JP 2003-99411       A  20030402
                                             WO 2004-JP4794      W  20040401

OTHER SOURCE(S):          CASREACT 141:350046
GI
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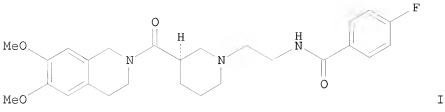


I

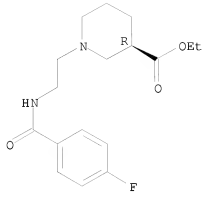
AB A novel crystal of (R)-(-)-N-[2-[3-[(6,7-dimethoxy-1,2,3,4-tetrahydroisoquinolin-2-yl)carbonyl]piperidino]ethyl]-4-fluorobenzamide (I) monophosphate, which is known as a preventive and/or remedy for ischemic diseases such as angina pectoris and myocardial infarction and cardiovascular diseases such as ischemic heart failure and arrhythmia, was prepared and characterized by X-ray diffraction spectra and DSC. Two crystal forms (α and β crystal forms) of compound I were prepared α Crystal form of compound I exhibited excellent moisture adsorption property and is advantageous for handling and formulation. Thus, 206.4 g (R)-1-[2-[(4-fluorobenzoyl)amino]ethyl]piperidine-3-carboxylic acid was treated with 810 mL DMF and 120.8 g 6,7-dimethoxy-1,2,3,4-tetrahydroisoquinoline monohydrochloride, stirred, cooled, treated with 53.22 g Et3N at ≤12°, treated with 217 mL DMF and then successively with 21.32 g 1H-1,2,3-benzotriazole and 121.0 g 1-ethyl-3-(3-dimethylaminopropyl)carbodiimide hydrochloride at ≤5°, and stirred at 0-4° for 15.5 h, and treated with 340 mL H2O, 2,000 mL EtOAc, and 550 mL 8% (W/V) aqueous NaOH solution to give, after workup and concentration, crude free base I (83.9% purity). I (11.90 g) was dissolved in ethanol to a total weight of 97.8 g, treated with 5 mL ethanol, 0.47 g H2O, and 0.86 g 85% H3PO4, and then with 5 mL ethanol, stirred at 30° overnight, and filtered to give, after washing the crystals with ethanol and drying, 3.38 g I monophosphate (α crystal form).

IT 721452-52-4P, (R)-1-[2-[(4-Fluorobenzoyl)amino]ethyl]piperidine-3-carboxylic acid ethyl ester 721452-55-7P, (R)-1-[2-[(4-Fluorobenzoyl)amino]ethyl]piperidine-3-carboxylic acid
RL: IMF (Industrial manufacture); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of novel crystal of fluorobenzamide monophosphate derivative having
excellent moisture adsorption property)

RN 721452-52-4 HCAPLUS

CN 3-Piperidinecarboxylic acid, 1-[2-[(4-fluorobenzoyl)amino]ethyl]-, ethyl ester, (3R)- (CA INDEX NAME)

Absolute stereochemistry.



RN 721452-55-7 HCAPLUS
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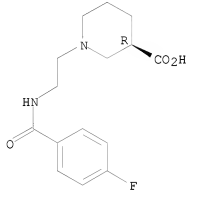
(CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 2 OF 2 HCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2004:565208 HCAPLUS
DOCUMENT NUMBER: 141:106387
TITLE: Isoquinoline derivatives containing benzamide moiety and process for their preparation
INVENTOR(S): Yoshida, Shinya; Watanabe, Toshihiro; Marumo, Kiyotaka; Kakefuda, Akio
PATENT ASSIGNEE(S): Yamanouchi Pharmaceutical Co., Ltd., Japan
SOURCE: PCT Int. Appl., 37 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.		DATE
WO 2004058710	A1	20040715	WO 2003-JP16582		20031224
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW					
RW: BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG					
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AU 2003292757	A1	20040722	AU 2003-292757		20031224
CN 1753870	A	20060329	CN 2003-80109919		20031224
IN 2005DN02787	A	20070105	IN 2005-DN2787		20050623
US 2006084807	A1	20060420	US 2005-540421		20050624
KR 758522	B1	20070914	KR 2005-711965		20050624
PRIORITY APPLN. INFO.:			JP 2002-375153	A	20021225
			WO 2003-JP16582	W	20031224
OTHER SOURCE(S):	MARPAT 141:106387				
GI					

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

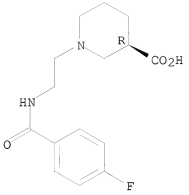
AB Process for the preparation of compds. I [R3 =, R4 = H, alkyl, alkoxy; Ar = (un)substituted aryl] and compds. II [R1 = H, alkyl, benzyl; R2 = H, protecting group of amino; Ar = (un)substituted aryl] were provided. For example, a mixture of compound (R)-II [R1 = Ethyl; R2 = H; Ar = 4-fluorophenyl] (37.94 g), e.g., prepared from (R)-piperidine-3-carboxylic acid Et ester L-tartaric acid salt in 4 steps, and 1 M aqueous NaOH (177 mL) in EtOH (100 mL) stirred at room temperature for 1 h. After treating the reaction with HCl to acidic pH, the solvent was azeotropically removed by toluene. Then, to a solution of the resulting residue in DMF (250 mL) were added 6,7-dimethoxy-1,2,3,4-tetrahydroisoquinoline hydrochloride (21.66 g), HOBt (7.97 g) and WSC hydrochloride (27.14 g) at 10 °C. The reaction was stirred at room temperature for 3 h, aqueous work-up followed by treatment with 85% phosphoric acid (13.65 g) in EtOH (500 mL) afforded claimed compound III phosphoric acid salt (44.25 g). Of note, compds. I are useful for prophylaxis and/or treatment of myocardial infarction, congestive heart failure, etc. (no data). The disclosed process employs less hazardous solvent.

IT 721452-55-7P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(N-benzoylaminoethylation of nipecotic acid derivs. using dihydrooxazoles)

RN 721452-55-7 HCAPLUS

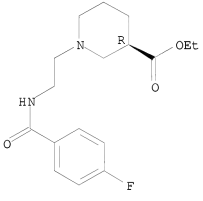
CN 3-Piperidinecarboxylic acid, 1-[2-[(4-fluorobenzoyl)amino]ethyl]-, (3R)- (CA INDEX NAME)

Absolute stereochemistry.



IT 721452-52-4P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of isoquinoline derivs. via N-fluorobenzoylation of tetrahydroisoquinoline derivs.)
RN 721452-52-4 HCAPLUS
CN 3-Piperidinecarboxylic acid, 1-[2-[(4-fluorobenzoyl)amino]ethyl]-, ethyl ester, (3R)- (CA INDEX NAME)

Absolute stereochemistry.



=> file caold

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	13.59	194.00
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	-1.60	-1.60

FILE 'CAOLD' ENTERED AT 22:15:22 ON 11 MAR 2008

10540421

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FILE COVERS 1907-1966
FILE LAST UPDATED:  01 May 1997 (19970501/UP)

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  assignees, and patent information, e.g., patent numbers, are
  now searchable from 1907-1966.  TIFF images of CA abstracts
  printed between 1907-1966 are available in the PAGE
  display formats.

  New CAS Information Use Policies, enter HELP USAGETERMS for details.

  This file supports REGistRY for direct browsing and searching of
  all substance data from the REGISTRY file.  Enter HELP FIRST for
  more information.

=> d his

     (FILE 'HOME' ENTERED AT 22:11:52 ON 11 MAR 2008)

     FILE 'REGISTRY' ENTERED AT 22:11:58 ON 11 MAR 2008
L1               STRUCTURE UPLOADED
L2            0 S L1
L3            2 S L1 FULL

     FILE 'HCAPLUS' ENTERED AT 22:14:49 ON 11 MAR 2008
L4            2 S L3
L5            0 S L4 AND SHINYA, Y?/AU
L6            2 S L4 AND WATANABE, T?/AU

     FILE 'CAOLD' ENTERED AT 22:15:22 ON 11 MAR 2008

=> s l3
L7            0 L3

=> file reg
COST IN U.S. DOLLARS                                SINCE FILE      TOTAL
                                                       ENTRY    SESSION
FULL ESTIMATED COST                                     0.46     194.46

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)          SINCE FILE      TOTAL
                                                       ENTRY    SESSION
CA SUBSCRIBER PRICE                                     0.00      -1.60

FILE 'REGISTRY' ENTERED AT 22:15:28 ON 11 MAR 2008
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provided by InfoChem.
```

10540421

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STRUCTURE FILE UPDATES:   10 MAR 2008  HIGHEST RN 1007341-18-5
DICTIONARY FILE UPDATES:  10 MAR 2008  HIGHEST RN 1007341-18-5

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH January 9, 2008.

  Please note that search-term pricing does apply when
  conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and
predicted properties as well as tags indicating availability of
experimental property data in the original document.  For information
on property searching in REGISTRY, refer to:

http://www.cas.org/support/stngen/stndoc/properties.html

=>
Uploading C:\Documents and Settings\brobinson1\My Documents\stnweb\Queries\421.str

L8      STRUCTURE UPLOADED

=> d 18
L8 HAS NO ANSWERS
L8              STR

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY -  AVAILABLE VIA OFFLINE PRINT *

Structure attributes must be viewed using STN Express query preparation.


=> s 18
SAMPLE SEARCH INITIATED 22:16:48 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED -      309 TO ITERATE

100.0% PROCESSED      309 ITERATIONS                                0 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:  ONLINE  **COMPLETE**
                        BATCH   **COMPLETE**
PROJECTED ITERATIONS:         5126 TO     7234
PROJECTED ANSWERS:               0 TO        0

L9            0 SEA SSS SAM L8

=> s 18 full
THE ESTIMATED SEARCH COST FOR FILE 'REGISTRY' IS 177.90 U.S. DOLLARS
DO YOU WANT TO CONTINUE WITH THIS REQUEST? (Y)/N or END:y
FULL SEARCH INITIATED 22:16:53 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED -     6564 TO ITERATE

100.0% PROCESSED     6564 ITERATIONS                               9 ANSWERS
SEARCH TIME: 00.00.01

L10           9 SEA SSS FUL L8
```

10540421

```
=> d his

     (FILE 'HOME' ENTERED AT 22:11:52 ON 11 MAR 2008)

     FILE 'REGISTRY' ENTERED AT 22:11:58 ON 11 MAR 2008
L1               STRUCTURE UPLOADED
L2            0 S L1
L3            2 S L1 FULL

     FILE 'HCAPLUS' ENTERED AT 22:14:49 ON 11 MAR 2008
L4            2 S L3
L5            0 S L4 AND SHINYA, Y?/AU
L6            2 S L4 AND WATANABE, T?/AU

     FILE 'CAOLD' ENTERED AT 22:15:22 ON 11 MAR 2008
L7            0 S L3

     FILE 'REGISTRY' ENTERED AT 22:15:28 ON 11 MAR 2008
L8               STRUCTURE UPLOADED
L9            0 S L8
L10           9 S L8 FULL

=> s l10 not l6
NUMERIC VALUE NOT VALID 'WATANABE, T?'
            0 WATANABE, T?/AU
L11           9 L10 NOT L6

=> file hcaplus
COST IN U.S. DOLLARS                                SINCE FILE      TOTAL
                                                       ENTRY    SESSION
FULL ESTIMATED COST                                    184.43     378.89

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)          SINCE FILE      TOTAL
                                                       ENTRY    SESSION
CA SUBSCRIBER PRICE                                      0.00      -1.60

FILE 'HCAPLUS' ENTERED AT 22:17:15 ON 11 MAR 2008
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FILE COVERS 1907 - 11 Mar 2008  VOL 148 ISS 11
FILE LAST UPDATED: 10 Mar 2008  (20080310/ED)

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This file contains CAS Registry Numbers for easy and accurate substance identification.

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=> s l11
L12          6 L11

=> s l12 and yoshida, s?/au
          9851 YOSHIDA, S?/AU
L13          2 L12 AND YOSHIDA, S?/AU

=> d l13, ibib abs hitstr, 1-6

L13  ANSWER 1 OF 2  HCAPLUS  COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER:         2004:872791  HCAPLUS
DOCUMENT NUMBER:          141:350046
TITLE:                    Preparation of novel crystal of fluorobenzamide
                          derivative
INVENTOR(S):              Yoshida, Shinya; Watanabe, Toshihiro;
                          Marumo, Kiyotaka; Yamaguchi, Sou
PATENT ASSIGNEE(S):       Yamanouchi Pharmaceutical Co., Ltd., Japan
SOURCE:                   PCT Int. Appl., 25 pp.
                          CODEN: PIXXD2
DOCUMENT TYPE:            Patent
LANGUAGE:                 Japanese
FAMILY ACC. NUM. COUNT:   1
PATENT INFORMATION:

     PATENT NO.          KIND   DATE        APPLICATION NO.         DATE
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     WO 2004089933        A1    20041021    WO 2004-JP4794          20040401
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             GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC,
             LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI,
             NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY,
             TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
         RW: BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ,
             BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE,
             ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI,
             SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN,
             TD, TG
     CA 2519882           A1    20041021    CA 2004-2519882         20040401
     EP 1609788           A1    20051228    EP 2004-725182          20040401
          R:  AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,
              IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, PL, SK, HR
     CN 1771245           A     20060510    CN 2004-80009451        20040401
     IN 2005DN04378       A     20070105    IN 2005-DN4378          20050927
     MX 2005PA10603       A     20060725    MX 2005-PA10603         20050930
     US 2007129357        A1    20070607    US 2005-552019          20051003
PRIORITY APPLN. INFO.:                       JP 2003-99411       A  20030402
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OTHER SOURCE(S):          CASREACT 141:350046
GI
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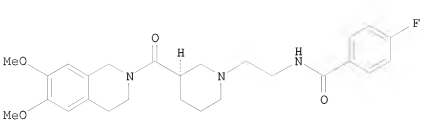


I

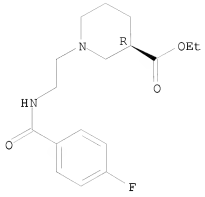
AB A novel crystal of (R)-(-)-N-[2-[3-[(6,7-dimethoxy-1,2,3,4-tetrahydroisoquinolin-2-yl)carbonyl]piperidino]ethyl]-4-fluorobenzamide (I) monophosphate, which is known as a preventive and/or remedy for ischemic diseases such as angina pectoris and myocardial infarction and cardiovascular diseases such as ischemic heart failure and arrhythmia, was prepared and characterized by X-ray diffraction spectra and DSC. Two crystal forms (α and β crystal forms) of compound I were prepared α Crystal form of compound I exhibited excellent moisture adsorption property and is advantageous for handling and formulation. Thus, 206.4 g (R)-1-[2-[(4-fluorobenzoyl)amino]ethyl]piperidine-3-carboxylic acid was treated with 810 mL DMF and 120.8 g 6,7-dimethoxy-1,2,3,4-tetrahydroisoquinoline monohydrochloride, stirred, cooled, treated with 53.22 g Et3N at ≤12°, treated with 217 mL DMF and then successively with 21.32 g 1H-1,2,3-benzotriazole and 121.0 g 1-ethyl-3-(3-dimethylaminopropyl)carbodiimide hydrochloride at ≤5°, and stirred at 0-4° for 15.5 h, and treated with 340 mL H2O, 2,000 mL EtOAc, and 550 mL 8% (W/V) aqueous NaOH solution to give, after workup and concentration, crude free base I (83.9% purity). I (11.90 g) was dissolved in ethanol to a total weight of 97.8 g, treated with 5 mL ethanol, 0.47 g H2O, and 0.86 g 85% H3PO4, and then with 5 mL ethanol, stirred at 30° overnight, and filtered to give, after washing the crystals with ethanol and drying, 3.38 g I monophosphate (α crystal form).

IT 721452-52-4P, (R)-1-[2-[(4-Fluorobenzoyl)amino]ethyl]piperidine-3-carboxylic acid ethyl ester 721452-55-7P, (R)-1-[2-[(4-Fluorobenzoyl)amino]ethyl]piperidine-3-carboxylic acid
RL: IMF (Industrial manufacture); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of novel crystal of fluorobenzamide monophosphate derivative having
excellent moisture adsorption property)

RN 721452-52-4 HCAPLUS

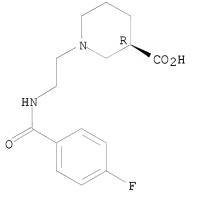
CN 3-Piperidinecarboxylic acid, 1-[2-[(4-fluorobenzoyl)amino]ethyl]-, ethyl ester, (3R)- (CA INDEX NAME)

Absolute stereochemistry.



RN 721452-55-7 HCAPLUS
CN 3-Piperidinecarboxylic acid, 1-[2-[(4-fluorobenzoyl)amino]ethyl]-, (3R)-
(CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L13 ANSWER 2 OF 2 HCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2004:565208 HCAPLUS
DOCUMENT NUMBER: 141:106387
TITLE: Isoquinoline derivatives containing benzamide moiety and process for their preparation
INVENTOR(S): Yoshida, Shinya; Watanabe, Toshihiro; Marumo, Kiyotaka; Kakefuda, Akio
PATENT ASSIGNEE(S): Yamanouchi Pharmaceutical Co., Ltd., Japan
SOURCE: PCT Int. Appl., 37 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.		DATE
WO 2004058710	A1	20040715	WO 2003-JP16582		20031224
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW					
RW: BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG					
CA 2511989	A1	20040715	CA 2003-2511989		20031224
AU 2003292757	A1	20040722	AU 2003-292757		20031224
CN 1753870	A	20060329	CN 2003-80109919		20031224
IN 2005DN02787	A	20070105	IN 2005-DN2787		20050623
US 2006084807	A1	20060420	US 2005-540421		20050624
KR 758522	B1	20070914	KR 2005-711965		20050624
PRIORITY APPLN. INFO.:			JP 2002-375153	A	20021225
			WO 2003-JP16582	W	20031224
OTHER SOURCE(S):	MARPAT 141:106387				
GI					

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

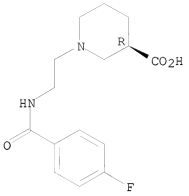
AB Process for the preparation of compds. I [R3 =, R4 = H, alkyl, alkoxy; Ar = (un)substituted aryl] and compds. II [R1 = H, alkyl, benzyl; R2 = H, protecting group of amino; Ar = (un)substituted aryl] were provided. For example, a mixture of compound (R)-II [R1 = Ethyl; R2 = H; Ar = 4-fluorophenyl] (37.94 g), e.g., prepared from (R)-piperidine-3-carboxylic acid Et ester L-tartaric acid salt in 4 steps, and 1 M aqueous NaOH (177 mL) in EtOH (100 mL) stirred at room temperature for 1 h. After treating the reaction with HCl to acidic pH, the solvent was azeotropically removed by toluene. Then, to a solution of the resulting residue in DMF (250 mL) were added 6,7-dimethoxy-1,2,3,4-tetrahydroisoquinoline hydrochloride (21.66 g), HOBt (7.97 g) and WSC hydrochloride (27.14 g) at 10 °C. The reaction was stirred at room temperature for 3 h, aqueous work-up followed by treatment with 85% phosphoric acid (13.65 g) in EtOH (500 mL) afforded claimed compound III phosphoric acid salt (44.25 g). Of note, compds. I are useful for prophylaxis and/or treatment of myocardial infarction, congestive heart failure, etc. (no data). The disclosed process employs less hazardous solvent.

IT 721452-55-7P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(N-benzoylaminoethylation of nipecotic acid derivs. using dihydrooxazoles)

RN 721452-55-7 HCAPLUS

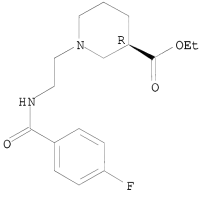
CN 3-Piperidinecarboxylic acid, 1-[2-[(4-fluorobenzoyl)amino]ethyl]-, (3R)- (CA INDEX NAME)

Absolute stereochemistry.



IT 721452-52-4P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of isoquinoline derivs. via N-fluorobenzoylation of tetrahydroisoquinoline derivs.)
RN 721452-52-4 HCAPLUS
CN 3-Piperidinecarboxylic acid, 1-[2-[(4-fluorobenzoyl)amino]ethyl]-, ethyl ester, (3R)- (CA INDEX NAME)

Absolute stereochemistry.



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L3 2 S L1 FULL

FILE 'HCAPLUS' ENTERED AT 22:14:49 ON 11 MAR 2008

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L5             0 S L4 AND SHINYA, Y?/AU
L6             2 S L4 AND WATANABE, T?/AU

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L7             0 S L3

     FILE 'REGISTRY' ENTERED AT 22:15:28 ON 11 MAR 2008
L8               STRUCTURE UPLOADED
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L18            2 L11/USES
                 (L11 (L) USES/RL)

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L18  ANSWER 1 OF 2  HCAPLUS  COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER:         2006:405003  HCAPLUS
DOCUMENT NUMBER:          146:155278
TITLE:                    Non-stochastic and stochastic linear indices of the
                          molecular pseudograph's atom-adjacency matrix: a novel
                          approach for computational in silico screening and
                          "rational" selection of new lead antibacterial agents
AUTHOR(S):                Marrero-Ponce, Yovani; Marrero, Ricardo Medina;
                          Torrens, Francisco; Martinez, Yamile; Bernal, Milagros
                          Garcia; Zaldivar, Vicente Romero; Castro, Eduardo A.;
                          Abalo, Ricardo Grau
CORPORATE SOURCE:         Department of Pharmacy, Faculty of Chemical-Pharmacy,
                          Central University of Las Villas, Santa Clara, 54830,
                          Cuba
SOURCE:                   Journal of Molecular Modeling (2006), 12(3), 255-271
                          CODEN: JMMOFK; ISSN: 0948-5023
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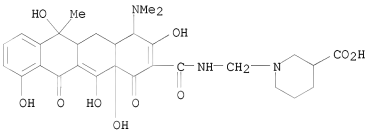
URL: http://www.springerlink.com/media/ef6tmfk36j3ttmb97wlh/contributions/l/2/v/4/l2v47qr26320v870.pdf
PUBLISHER: Springer GmbH
DOCUMENT TYPE: Journal; (online computer file)
LANGUAGE: English

AB A novel approach (TOMOCOMD-CARDD) to computer-aided rational drug design is illustrated. This approach is based on the calcn. of the non-stochastic and stochastic linear indexes of the mol. pseudograph's atom-adjacency matrix representing mol. structures. These TOMOCOMD-CARDD descriptors are introduced for the computational (virtual) screening and rational selection of new lead antibacterial agents using linear discrimination anal. The two structure-based antibacterial-activity classification models, including non-stochastic and stochastic indexes, classify correctly 91.61% and 90.75%, resp., of 1525 chems. in training sets. These models show high Matthews correlation coeffs. (MCC = 0.84 and 0.82). An external validation process was carried out to assess the robustness and predictive power of the model obtained. These QSAR models permit the correct classification of 91.49% and 89.31% of 505 compds. in an external test set, yielding MCCs of 0.84 and 0.79, resp. The TOMOCOMD-CARDD approach compares satisfactorily with respect to nine of the most useful models for antimicrobial selection reported to date. Finally, an in silico screening of 87 new chems. reported in the antiinfective field with antibacterial activities is developed showing the ability of the TOMOCOMD-CARDD models to identify new lead antibacterial compds.

IT 15301-82-3, Pecocycline
RL: PAC (Pharmacological activity); PRP (Properties); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(novel QSAR model TOMOCOMD-CARDD in computer-aided rational drug design for selection of new lead antibacterial agents using linear discrimination anal.)

RN 15301-82-3 HCAPLUS

CN 3-Piperidinecarboxylic acid, (4S,4aS,5aS,6S,12aS)-1-[[[[4-(dimethylamino)-1,4,4a,5,5a,6,11,12a-octahydro-3,6,10,12,12a-pentahydroxy-6-methyl-1,11-dioxo-2-naphthacenyl]carbonyl]amino]methyl]- (CA INDEX NAME)



REFERENCE COUNT: 71 THERE ARE 71 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L18 ANSWER 2 OF 2 HCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2005:244333 HCAPLUS
DOCUMENT NUMBER: 143:307
TITLE: Atom, atom-type, and total nonstochastic and stochastic quadratic fingerprints: a promising

approach for modeling of antibacterial activity

AUTHOR(S): Marrero-Ponce, Yovani; Medina-Marrero, Ricardo; Torrens, Francisco; Martinez, Yamile; Romero-Zaldivar, Vicente; Castro, Eduardo A.

CORPORATE SOURCE: Department of Pharmacy, Faculty of Chemical-Pharmacy, Central University of Las Villas, Santa Clara, 54830, Cuba

SOURCE: Bioorganic & Medicinal Chemistry (2005), 13(8), 2881-2899
CODEN: BMECEP; ISSN: 0968-0896

PUBLISHER: Elsevier Ltd.

DOCUMENT TYPE: Journal

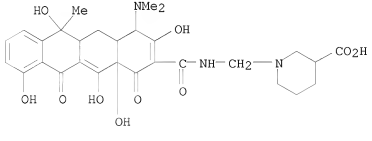
LANGUAGE: English

AB The Topol. Mol. Computer Design (TOMOCOMD-CARDD) approach has been introduced for the classification and design of antimicrobial agents using computer-aided mol. design. For this propose, atom, atom-type, and total quadratic indexes have been generalized to codify chemical structure information. In this sense, stochastic quadratic indexes have been introduced for the description of the mol. structure. These stochastic fingerprints are based on a simple model for the intramol. movement of all valence-bond electrons. In this work, a complete data set containing 1006 antimicrobial agents is collected and presented. Two structure-based antibacterial activity classification models have been generated. The models (including nonstochastic and stochastic indexes) classify correctly more than 90% of 1525 compds. in training sets. These models permit the correct classification of 92.28% and 89.31% of 505 compds. in an external test sets. The approach, also, satisfactorily compares with respect to nine of the most useful models for antimicrobial selection reported to date. Finally, a virtual screening of 87 new compds. reported in the anti-infective field with antibacterial activities is developed showing the ability of the models to identify new leads as antibacterial.

IT 15301-82-3, Pecocycline
RL: PAC (Pharmacological activity); PRP (Properties); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(atom, atom-type, and total nonstochastic and stochastic quadratic fingerprints as promising approach for modeling antibacterial activity)

RN 15301-82-3 HCAPLUS

CN 3-Piperidinecarboxylic acid, (4S,4aS,5aS,6S,12aS)-1-[[[[4-(dimethylamino)-1,4,4a,5,5a,6,11,12a-octahydro-3,6,10,12,12a-pentahydroxy-6-methyl-1,11-dioxo-2-naphthacenyl]carbonyl]amino]methyl]- (CA INDEX NAME)



REFERENCE COUNT: 91 THERE ARE 91 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

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L3             2 S L1 FULL

     FILE 'HCAPLUS' ENTERED AT 22:14:49 ON 11 MAR 2008
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L5             0 S L4 AND SHINYA, Y?/AU
L6             2 S L4 AND WATANABE, T?/AU

     FILE 'CAOLD' ENTERED AT 22:15:22 ON 11 MAR 2008
L7             0 S L3

     FILE 'REGISTRY' ENTERED AT 22:15:28 ON 11 MAR 2008
L8             STRUCTURE UPLOADED
L9             0 S L8
L10            9 S L8 FULL
L11            9 S L10 NOT L6

     FILE 'HCAPLUS' ENTERED AT 22:17:15 ON 11 MAR 2008
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L13            2 S L12 AND YOSHIDA, S?/AU
L14            4 S L12 NOT L13
L15            0 S L14 AND WATANABE, T?/AU
L16            0 S L14 AND MARUMO, K?/AU
L17            0 S L14 AND KAKEFUDA, A?/AU
L18            2 S L11/USES

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                                                       ENTRY    SESSION
FULL ESTIMATED COST                                    29.87     408.76

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)          SINCE FILE      TOTAL
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CA SUBSCRIBER PRICE                                    -3.20      -4.80

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FILE COVERS 1907-1966
FILE LAST UPDATED:  01 May 1997 (19970501/UP)

  This file contains CAS Registry Numbers for easy and accurate
  substance identification.  Title keywords, authors, patent
  assignees, and patent information, e.g., patent numbers, are
  now searchable from 1907-1966.  TIFF images of CA abstracts
  printed between 1907-1966 are available in the PAGE
  display formats.
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This file supports REGlstRY for direct browsing and searching of all substance data from the REGISTRY file. Enter HELP FIRST for more information.

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L19           1 L11

=> d l19, all, 1

L19  ANSWER 1 OF 1  CAOLD  COPYRIGHT 2008 ACS on STN
AN   CA63:13180h  CAOLD
TI   pyrenylmethylamines
AU   Clarke, Robert LaGrone; Buck, J. S.
PA   Sterling Drug Inc.
DT   Patent
     PATENT NO.    KIND          DATE
     ------------  -----------   ----
PI   US 3198835                  1965
IT     897-41-6    1729-05-1     3590-94-1    3590-95-2    3590-96-3
     3590-97-4     3590-98-5     3590-99-6    3591-00-2    3591-01-3    3591-02-4
     3591-03-5     3712-78-5     3712-79-6    3765-68-2    3786-54-7    3786-55-8
     3786-56-9     3786-57-0     3786-59-2    3786-60-5    3786-61-6    3786-62-7
     3786-63-8     3786-66-1     3786-67-2    3804-54-4    3804-55-5    3806-02-8
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CA SUBSCRIBER PRICE                                     0.00      -4.80

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STRUCTURE FILE UPDATES:   10 MAR 2008  HIGHEST RN 1007341-18-5
DICTIONARY FILE UPDATES:  10 MAR 2008  HIGHEST RN 1007341-18-5

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  Please note that search-term pricing does apply when
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conducting SmartSELECT searches.

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http://www.cas.org/support/stngen/stndoc/properties.html

=> S 6614-22-8/RN

L20 1 6614-22-8/RN

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NOTICE SET TO 1 U.S. DOLLAR FOR DISPLAY COMMAND
SET COMMAND COMPLETED

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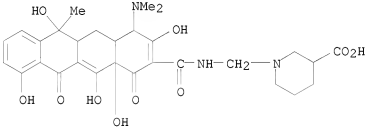
YOU HAVE REQUESTED DATA FROM 1 ANSWERS - CONTINUE? Y/(N):y
THE ESTIMATED COST FOR THIS REQUEST IS 6.65 U.S. DOLLARS
DO YOU WANT TO CONTINUE WITH THIS REQUEST? (Y)/N:y

L20 ANSWER 1 OF 1 REGISTRY COPYRIGHT 2008 ACS on STN
RN 6614-22-8 REGISTRY
CN Nipecotic acid, 1-[[4-(dimethylamino)-1,4,4a,5,5a,6,11,12a-octahydro-3,6,10,12,12a-pentahydroxy-6-methyl-1,11-dioxo-2-naphthacenecarboxamido]methyl]-, hydrochloride (7CI, 8CI) (CA INDEX NAME)
MF C29 H35 N3 O10 . Cl H
LC STN Files: CA, CAOLD, CAPLUS, USPATOLD
DT.CA CAplus document type: Patent
RL.P Roles from patents: PREP (Preparation)
CRN (741608-18-4)



● HCl

2 REFERENCES IN FILE CA (1907 TO DATE)
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1 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

10540421

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SET COMMAND COMPLETED

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COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	2.46	412.83

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CA SUBSCRIBER PRICE	0.00	-4.80

FILE 'REGISTRY' ENTERED AT 22:20:39 ON 11 MAR 2008
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Property values tagged with IC are from the ZIC/VINITI data file
provided by InfoChem.

STRUCTURE FILE UPDATES: 10 MAR 2008 HIGHEST RN 1007341-18-5
DICTIONARY FILE UPDATES: 10 MAR 2008 HIGHEST RN 1007341-18-5

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH January 9, 2008.

  Please note that search-term pricing does apply when
  conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and
predicted properties as well as tags indicating availability of
experimental property data in the original document. For information
on property searching in REGISTRY, refer to:

http://www.cas.org/support/stngen/stndoc/properties.html

=>
Uploading C:\Documents and Settings\brobinson1\My Documents\stnweb\Queries\2ef.str

L21   STRUCTURE UPLOADED

=> d l21
L21 HAS NO ANSWERS
L21   STR

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

Structure attributes must be viewed using STN Express query preparation.

=> s l21

Updated Search

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SAMPLE SEARCH INITIATED 22:21:53 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED -     8538 TO ITERATE

 23.4% PROCESSED     2000 ITERATIONS                                0 ANSWERS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:  ONLINE  **COMPLETE**
                        BATCH   **COMPLETE**
PROJECTED ITERATIONS:       165221 TO   176299
PROJECTED ANSWERS:               0 TO        0

L22           0 SEA SSS SAM L21

=> s l21 full
THE ESTIMATED SEARCH COST FOR FILE 'REGISTRY' IS 177.90 U.S. DOLLARS
DO YOU WANT TO CONTINUE WITH THIS REQUEST? (Y)/N or END:y
FULL SEARCH INITIATED 22:21:57 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED -   170590 TO ITERATE

100.0% PROCESSED   170590 ITERATIONS                               3 ANSWERS
SEARCH TIME: 00.00.03

L23           3 SEA SSS FUL L21

=> d his

     (FILE 'HOME' ENTERED AT 22:11:52 ON 11 MAR 2008)

     FILE 'REGISTRY' ENTERED AT 22:11:58 ON 11 MAR 2008
L1              STRUCTURE UPLOADED
L2            0 S L1
L3            2 S L1 FULL

     FILE 'HCAPLUS' ENTERED AT 22:14:49 ON 11 MAR 2008
L4            2 S L3
L5            0 S L4 AND SHINYA, Y?/AU
L6            2 S L4 AND WATANABE, T?/AU

     FILE 'CAOLD' ENTERED AT 22:15:22 ON 11 MAR 2008
L7            0 S L3

     FILE 'REGISTRY' ENTERED AT 22:15:28 ON 11 MAR 2008
L8              STRUCTURE UPLOADED
L9            0 S L8
L10           9 S L8 FULL
L11           9 S L10 NOT L6

     FILE 'HCAPLUS' ENTERED AT 22:17:15 ON 11 MAR 2008
L12           6 S L11
L13           2 S L12 AND YOSHIDA, S?/AU
L14           4 S L12 NOT L13
L15           0 S L14 AND WATANABE, T?/AU
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     FILE 'CAOLD' ENTERED AT 22:18:56 ON 11 MAR 2008
L19             1 S L11

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L20             1 S 6614-22-8/RN
                  SET NOTICE 1 DISPLAY
                  SET NOTICE LOGIN DISPLAY

     FILE 'REGISTRY' ENTERED AT 22:20:39 ON 11 MAR 2008
L21               STRUCTURE UPLOADED
L22             0 S L21
L23             3 S L21 FULL

=> s l23 not l3
L24             1 L23 NOT L3

=> s l24 not l11
L25             1 L24 NOT L11

=> s l24 not l18
'USES' IS NOT A VALID CROSSOVER QUALIFIER FOR L11
Answer sets created in a different file may be field qualified with a
limited set of qualifiers.  Enter HELP CROSSOVER at an arrow prompt
(=>) for specific information.

=> file hcaplus
COST IN U.S. DOLLARS                                SINCE FILE      TOTAL
                                                       ENTRY    SESSION
FULL ESTIMATED COST                                   179.28     592.11

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)          SINCE FILE      TOTAL
                                                       ENTRY    SESSION
CA SUBSCRIBER PRICE                                     0.00      -4.80

FILE 'HCAPLUS' ENTERED AT 22:22:31 ON 11 MAR 2008
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FILE COVERS 1907 - 11 Mar 2008  VOL 148 ISS 11
FILE LAST UPDATED: 10 Mar 2008  (20080310/ED)

New CAS Information Use Policies, enter HELP USAGETERMS for details.
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This file contains CAS Registry Numbers for easy and accurate substance identification.

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L27           0 L26 AND YOSHIDA, S?/AU

=> s l26 and watanabe, t?/au
         22474 WATANABE, T?/AU
L28           0 L26 AND WATANABE, T?/AU

=> s l26 and marumo, k?/au
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=> s l26 and  kakefuda, a?/au
            45 KAKEFUDA, A?/AU
L30           0 L26 AND  KAKEFUDA, A?/AU

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L26  ANSWER 1 OF 2  HCAPLUS  COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER:         2006:1228883  HCAPLUS
DOCUMENT NUMBER:          145:505447
TITLE:                    Preparation of high-conductance, calcium-sensitive
                          potassium channel openers
INVENTOR(S):              Imanishi, Yasuhiro; Awai, Nobumasa; Hirai, Miki;
                          Hosaka, Toshihiro; Kono, Rikako
PATENT ASSIGNEE(S):       Tanabe Seiyaku Co., Ltd., Japan
SOURCE:                   Jpn. Kokai Tokkyo Koho, 164pp.
                          CODEN: JKXXAF
DOCUMENT TYPE:            Patent
LANGUAGE:                 Japanese
FAMILY ACC. NUM. COUNT:   1
PATENT INFORMATION:

     PATENT NO.          KIND   DATE        APPLICATION NO.        DATE
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     JP 2006316054        A     20061124    JP 2006-111427         20060414
PRIORITY APPLN. INFO.:                      JP 2005-117662      A  20050415
OTHER SOURCE(S):          MARPAT 145:505447
GI
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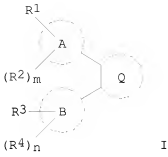


I

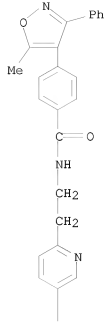
AB Title openers, useful for prophylactic and therapeutic treatment of urinary frequency, incontinence, asthma, and chronic obstructive pulmonary disease, are prepared from tricyclic compds. I [ring A = benzene, heterocycle; ring B = benzene, heterocycle, cycloalkane, cycloalkene; ring Q = halo- or (halo)alkyl-substituted pyrazole, isoxazole; R1, R3 = R5R6NCO, R5ONR6CO, R5R6NNHCO, R5CO, R5O, R5S, H, etc; R2, R4 = O, cyano, NO2, OH, alkoxy, halo, CO2H, etc.; R5, R6 = H, (un)substituted alkyl, (condensed) (un)substituted cycloalkyl, (un)substituted heterocyclyl, etc.; m, n = 0-2] are prepared Thus, deprotection of BOC-protected pyrazole derivative II (R = BOC) gave II (R = H), which inhibited K-induced bladder contraction with IC50 value of 1-3 μM.

IT 850832-10-9P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of pyrazoles or isoxazoles as high-conductance, Ca2+-sensitive K+ channel openers for treatment of diseases)

RN 850832-10-9 HCAPLUS

CN 3-Pyridinecarboxylic acid, 6-[2-[[4-(5-methyl-3-phenyl-4-isoxazolyl)benzoyl]amino]ethyl]-, ethyl ester (CA INDEX NAME)

PAGE 1-A



PAGE 2-A

L26 ANSWER 2 OF 2 HCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2005:369275 HCAPLUS
DOCUMENT NUMBER: 142:430265
TITLE: Preparation of substituted pyrazoles and isoxazoles as large conductance Ca-activated K channel openers
INVENTOR(S): Imanishi, Yasuhiro; Awai, Nobumasa; Hirai, Miki; Hosaka, Toshihiro; Kono, Rikako
PATENT ASSIGNEE(S): Tanabe Seiyaku Co., Ltd., Japan
SOURCE: PCT Int. Appl., 224 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005037271	A2	20050428	WO 2004-JP15662	20041015
WO 2005037271	A3	20050901		

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RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

EP 1675585 A2 20060705 EP 2004-792804 20041015
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US 2007060629 A1 20070315 US 2006-574529 20060404
PRIORITY APPLN. INFO.: JP 2003-357325 A 20031017
JP 2004-17662 A 20040126
JP 2004-85143 A 20040323
JP 2004-194172 A 20040630
US 2004-584451P P 20040701
WO 2004-JP15662 W 20041015

OTHER SOURCE(S): CASREACT 142:430265; MARPAT 142:430265

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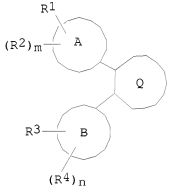


I

AB Title compds. I [A = benzene, heterocycle; B = benzene, heterocycle, etc.; Q = pyrazolyl, isoxazolyl; R1, R3 = carboxamido, hydrazido, etc.; m, n = 0-2; R2, R4 = oxo, CN, NO2, etc.] are prepared For instance, 4,4,4-trifluoro-1-(4-methylphenyl)butane-1,3-dione is reacted with 3-methylphenylhydrazine•HCl (EtOH, reflux, 20 h) to give 1-(3-methylphenyl)-5-(4-methylphenyl)-3-(trifluoromethyl)-1H-pyrazole (II). Data for over 400 compds. is given. The relaxation effect on K-induced contraction of isolated rabbit urinary bladder and the inhibitory effect on the rhythmic bladder contractions induced by substance P in anesthetized rats is provided for selected example compds. I are useful for the treatment of pollakiuria, urinary incontinence, etc.

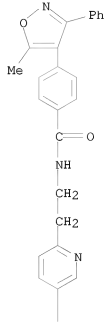
IT 850832-10-9P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of substituted pyrazoles and isoxazoles as large conductance Ca-activated K channel openers)

RN 850832-10-9 HCAPLUS

CN 3-Pyridinecarboxylic acid, 6-[2-[[4-(5-methyl-3-phenyl-4-isoxazolyl)benzoyl]amino]ethyl]-, ethyl ester (CA INDEX NAME)

PAGE 1-A



PAGE 2-A

=> file caold

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	13.59	605.70
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	-1.60	-6.40

Updated Search

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FILE COVERS 1907-1966
FILE LAST UPDATED:  01 May 1997 (19970501/UP)

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  assignees, and patent information, e.g., patent numbers, are
  now searchable from 1907-1966.  TIFF images of CA abstracts
  printed between 1907-1966 are available in the PAGE
  display formats.

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=> d his

     (FILE 'HOME' ENTERED AT 22:11:52 ON 11 MAR 2008)

     FILE 'REGISTRY' ENTERED AT 22:11:58 ON 11 MAR 2008
L1               STRUCTURE UPLOADED
L2            0 S L1
L3            2 S L1 FULL

     FILE 'HCAPLUS' ENTERED AT 22:14:49 ON 11 MAR 2008
L4            2 S L3
L5            0 S L4 AND SHINYA, Y?/AU
L6            2 S L4 AND WATANABE, T?/AU

     FILE 'CAOLD' ENTERED AT 22:15:22 ON 11 MAR 2008
L7            0 S L3

     FILE 'REGISTRY' ENTERED AT 22:15:28 ON 11 MAR 2008
L8               STRUCTURE UPLOADED
L9            0 S L8
L10           9 S L8 FULL
L11           9 S L10 NOT L6

     FILE 'HCAPLUS' ENTERED AT 22:17:15 ON 11 MAR 2008
L12           6 S L11
L13           2 S L12 AND YOSHIDA, S?/AU
L14           4 S L12 NOT L13
L15           0 S L14 AND WATANABE, T?/AU
L16           0 S L14 AND MARUMO, K?/AU
L17           0 S L14 AND KAKEFUDA, A?/AU
L18           2 S L11/USES

     FILE 'CAOLD' ENTERED AT 22:18:56 ON 11 MAR 2008
L19           1 S L11
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     FILE 'REGISTRY' ENTERED AT 22:19:57 ON 11 MAR 2008
L20             1 S 6614-22-8/RN
                  SET NOTICE 1 DISPLAY
                  SET NOTICE LOGIN DISPLAY

     FILE 'REGISTRY' ENTERED AT 22:20:39 ON 11 MAR 2008
L21               STRUCTURE UPLOADED
L22             0 S L21
L23             3 S L21 FULL
L24             1 S L23 NOT L3
L25             1 S L24 NOT L11

     FILE 'HCAPLUS' ENTERED AT 22:22:31 ON 11 MAR 2008
L26             2 S L25
L27             0 S L26 AND YOSHIDA, S?/AU
L28             0 S L26 AND WATANABE, T?/AU
L29             0 S L26 AND MARUMO, K?/AU
L30             0 S L26 AND  KAKEFUDA, A?/AU

     FILE 'CAOLD' ENTERED AT 22:23:23 ON 11 MAR 2008

=> s l25
L31             0 L25

=> file hcaplus
COST IN U.S. DOLLARS                                SINCE FILE      TOTAL
                                                       ENTRY    SESSION
FULL ESTIMATED COST                                     0.46     606.16

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)          SINCE FILE      TOTAL
                                                       ENTRY    SESSION
CA SUBSCRIBER PRICE                                     0.00      -6.40

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FILE COVERS 1907 - 11 Mar 2008  VOL 148 ISS 11
FILE LAST UPDATED: 10 Mar 2008  (20080310/ED)

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substance identification.

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=> d his

     (FILE 'HOME' ENTERED AT 22:11:52 ON 11 MAR 2008)

     FILE 'REGISTRY' ENTERED AT 22:11:58 ON 11 MAR 2008
L1             STRUCTURE UPLOADED
L2           0 S L1
L3           2 S L1 FULL

     FILE 'HCAPLUS' ENTERED AT 22:14:49 ON 11 MAR 2008
L4           2 S L3
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L8             STRUCTURE UPLOADED
L9           0 S L8
L10          9 S L8 FULL
L11          9 S L10 NOT L6

     FILE 'HCAPLUS' ENTERED AT 22:17:15 ON 11 MAR 2008
L12          6 S L11
L13          2 S L12 AND YOSHIDA, S?/AU
L14          4 S L12 NOT L13
L15          0 S L14 AND WATANABE, T?/AU
L16          0 S L14 AND MARUMO, K?/AU
L17          0 S L14 AND KAKEFUDA, A?/AU
L18          2 S L11/USES

     FILE 'CAOLD' ENTERED AT 22:18:56 ON 11 MAR 2008
L19          1 S L11

     FILE 'REGISTRY' ENTERED AT 22:19:57 ON 11 MAR 2008
L20          1 S 6614-22-8/RN
               SET NOTICE 1 DISPLAY
               SET NOTICE LOGIN DISPLAY

     FILE 'REGISTRY' ENTERED AT 22:20:39 ON 11 MAR 2008
L21            STRUCTURE UPLOADED
L22          0 S L21
L23          3 S L21 FULL
L24          1 S L23 NOT L3
L25          1 S L24 NOT L11

     FILE 'HCAPLUS' ENTERED AT 22:22:31 ON 11 MAR 2008
L26          2 S L25
L27          0 S L26 AND YOSHIDA, S?/AU
L28          0 S L26 AND WATANABE, T?/AU
L29          0 S L26 AND MARUMO, K?/AU
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     FILE 'HCAPLUS' ENTERED AT 22:23:39 ON 11 MAR 2008

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                 (L25 (L) USES/RL)

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L32  ANSWER 1 OF 2  HCAPLUS  COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER:         2006:1228883  HCAPLUS
DOCUMENT NUMBER:          145:505447
TITLE:                    Preparation of high-conductance, calcium-sensitive
                          potassium channel openers
INVENTOR(S):              Imanishi, Yasuhiro; Awai, Nobumasa; Hirai, Miki;
                          Hosaka, Toshihiro; Kono, Rikako
PATENT ASSIGNEE(S):       Tanabe Seiyaku Co., Ltd., Japan
SOURCE:                   Jpn. Kokai Tokkyo Koho, 164pp.
                          CODEN: JKXXAF
DOCUMENT TYPE:            Patent
LANGUAGE:                 Japanese
FAMILY ACC. NUM. COUNT:   1
PATENT INFORMATION:

     PATENT NO.          KIND   DATE        APPLICATION NO.          DATE
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     JP 2006316054        A     20061124    JP 2006-111427           20060414
PRIORITY APPLN. INFO.:                      JP 2005-117662      A    20050415
OTHER SOURCE(S):          MARPAT 145:505447
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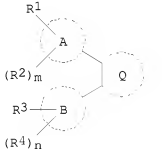


I

AB Title openers, useful for prophylactic and therapeutic treatment of urinary frequency, incontinence, asthma, and chronic obstructive pulmonary disease, are prepared from tricyclic compds. I [ring A = benzene, heterocycle; ring B = benzene, heterocycle, cycloalkane, cycloalkene; ring

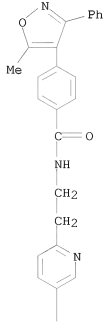
Q = halo- or (halo)alkyl-substituted pyrazole, isoxazole; R1, R3 = R5R6NCO, R5ONR6CO, R5R6NNHCO, R5CO, R5O, R5S, H, etc; R2, R4 = O, cyano, NO2, OH, alkoxy, halo, CO2H, etc.; R5, R6 = H, (un)substituted alkyl, (condensed) (un)substituted cycloalkyl, (un)substituted heterocyclyl, etc.; m, n = 0-2] are prepared Thus, deprotection of BOC-protected pyrazole derivative II (R = BOC) gave II (R = H), which inhibited K-induced bladder contraction with IC50 value of 1-3 μM.

IT 850832-10-9P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of pyrazoles or isoxazoles as high-conductance, Ca2+-sensitive K+ channel openers for treatment of diseases)

RN 850832-10-9 HCAPLUS

CN 3-Pyridinecarboxylic acid, 6-[2-[[4-(5-methyl-3-phenyl-4-isoxazolyl)benzoyl]amino]ethyl]-, ethyl ester (CA INDEX NAME)

PAGE 1-A



PAGE 2-A

L32 ANSWER 2 OF 2 HCAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2005:369275 HCAPLUS
DOCUMENT NUMBER: 142:430265
TITLE: Preparation of substituted pyrazoles and isoxazoles as large conductance Ca-activated K channel openers
INVENTOR(S): Imanishi, Yasuhiro; Awai, Nobumasa; Hirai, Miki; Hosaka, Toshihiro; Kono, Rikako
PATENT ASSIGNEE(S): Tanabe Seiyaku Co., Ltd., Japan
SOURCE: PCT Int. Appl., 224 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.		DATE
WO 2005037271	A2	20050428	WO 2004-JP15662		20041015
WO 2005037271	A3	20050901			
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EP 1675585	A2	20060705	EP 2004-792804		20041015
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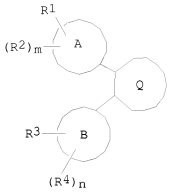
US 2007060629	A1	20070315	US 2006-574529		20060404
PRIORITY APPLN. INFO.:			JP 2003-357325	A	20031017
			JP 2004-17662	A	20040126
			JP 2004-85143	A	20040323
			JP 2004-194172	A	20040630
			US 2004-584451P	P	20040701
			WO 2004-JP15662	W	20041015

OTHER SOURCE(S): CASREACT 142:430265; MARPAT 142:430265
GI



I

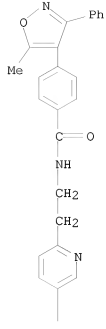
AB Title compds. I [A = benzene, heterocycle; B = benzene, heterocycle, etc.; Q = pyrazolyl, isoxazolyl; R1, R3 = carboxamido, hydrazido, etc.; m, n = 0-2; R2, R4 = oxo, CN, NO2, etc.] are prepared For instance, 4,4,4-trifluoro-1-(4-methylphenyl)butane-1,3-dione is reacted with 3-methylphenylhydrazine•HCl (EtOH, reflux, 20 h) to give 1-(3-methylphenyl)-5-(4-methylphenyl)-3-(trifluoromethyl)-1H-pyrazole (II). Data for over 400 compds. is given. The relaxation effect on K-induced contraction of isolated rabbit urinary bladder and the inhibitory effect on the rhythmic bladder contractions induced by substance P in anesthetized rats is provided for selected example compds. I are useful for the treatment of pollakiuria, urinary incontinence, etc.

IT 850832-10-9P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of substituted pyrazoles and isoxazoles as large conductance Ca-activated K channel openers)

RN 850832-10-9 HCAPLUS

CN 3-Pyridinecarboxylic acid, 6-[2-[[4-(5-methyl-3-phenyl-4-isoxazolyl)benzoyl]amino]ethyl]-, ethyl ester (CA INDEX NAME)

PAGE 1-A



PAGE 2-A